Methyl 4-hydroxy(²H₄)benzoate 362049-51-2 | DTXSID20858080

Model Performance			
N	Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 1.12e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.78e-01

Confidence level: 3.95e-01

Nearest Neighbors from the Training Set

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2,6-Diethylaniline Measured: 1.59e-05 Predicted: 2.02e-02

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Butyl phenyl ether Measured: 1.08e-03 Predicted: 5.92e-01

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2-Methoxyprop-1-ene Measured: 8.46e-02 Predicted: 474

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4-(2,4-Dinitroanilino)phenol

Measured: 3.43e-02 Predicted: 1.31e-11